Simulating geographically distributed production networks of a climate neutral European petrochemical industry

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Abstract
The paper describes quantitative scenarios on a possible evolution of the EU petrochemical industry towards climate neutrality. This industry will be one of the remaining sectors in a climate neutral economy still handling hydrocarbon material to manufacture polymers. Concepts of a climate neutral chemical industry stress the need to consider the potential end-of-life emissions of polymers produced from fossil feedstock and draft the vision of using renewable electricity to produce hydrogen and to use renewable (hydro)carbon feedstock. The latter could be biomass, CO_2 from the air or recycled feedstock from plastic waste streams.

The cost-optimization model used to develop the scenarios describes at which sites investments of industry in the production stock could take place in the future. Around 50 types of products, the related production processes and the respective sites have been collected in a database. The processes included cover the production chain from platform chemicals via intermediates to polymers. Pipelines allowing for efficient exchange of feedstock and platform chemicals between sites are taken into account as well. The model draws on this data to simulate capacity change at individual plants as well as plant utilization. Thus, a future European production network for petrochemicals with flows between the different sites and steps of the value chain can be sketched.

The scenarios described in this paper reveal how an electrification strategy could be implemented by European industry over time with minimized societal costs. Today's existing assets as well as geographical variance of energy supply and the development of demand for different plastic sorts are the major model drivers.

Finally, implications for the chemical industry, the energy system and national or regional governments are discussed.

Introduction
The chemical industry is one of the major energy consuming sectors in the European energy system. According to Eurostat's (2020) energy balance for the year 2018 its final energy demand makes up to 2.2 EJ, which is 20 % of the whole manufacturing sector. Non-energy use is even more relevant and amounts to 4 EJ. The petrochemical industry is the part of this industry dealing with organic materials. Today, mainly crude oil derived feedstock is processed in this industry. The main product of this branch are polymers, and these are mainly used as plastics for packaging, the automotive industry and the construction sector (PlasticsEurope 2019).

Worldwide, the production of plastics is rapidly growing (PlasticsEurope 2019). The share of the chemical industry in the use of oil products is growing as well (IEA 2018a). With the need to de-fossilize transport fuels in ambitious climate protection scenarios many studies see the petrochemical industry as the main user of oil feedstock in the future (IEA 2018b).

De-fossilization is however also at stake for the feedstock as all carbon used as a feedstock will at some point in time be emitted to the atmosphere. Applying carbon capture and storage (CCS) when incinerating plastic waste at the end of product lifetime may fix that problem to some degree from a CO_2 mitigation perspective. The total carbon capture rate depends on three parameters: (1) rate of carbon capture realized by collecting the waste, (2) adoption rate of CCS, and (3) technical CO_2 capture rate achieved in the incineration process itself. However, a 100 % total carbon capture rate cannot be achieved due to limitations at each of the three levels.

Going for carbon neutrality therefore requires a change in feedstock and moving away from crude oil. Not all recent scenario studies did however take that into account (see e.g. Boulamanti et al. 2017). However, the chemical industry acknowledges the need for such a shift in general. Whereas the 2013 version of the roadmap developed by the European Association of the chemical industry (CEFIC 2013) did not provide scenarios showing full GHG neutrality this has changed remarkably since the adoption of the Paris agreement. The recent roadmaps of the German and Dutch associations of the chemical industry (VCI 2019, VNCI 2018) explicitly consider the end-of-life (EOL) emissions of their products and thus acknowledge the responsibility to address them to achieve full neutrality. In the language of life cycle analysis such an emission scope is referred to as "scope 3 emissions".

A thorough approach will thus require the feedstock to be climate neutral from the beginning, i.e. it should not be derived from a fossil source. Alternative hydrocarbon sources substituting fossil crude oil could be biomass, recycled feedstock from plastic waste streams or CO_2 from the air. Activating CO_2 requires large amounts of additional hydrogen and energy. If other carbon sources like biomass or plastic waste are used (which already contain hydrogen) the carbon utilization rate may be boosted by additional hydrogen as well.

Energy demand is however not limited to feedstock use. The production chain from feedstock to polymer is often complex and involves in some chains several intermediate products. The processing requires thermal energy and sometimes the use of reactants like chlorine. Thus, the energy demand of processing in the petrochemical industry is considerable as well. According to our calculations thermal energy demand in year 2016 amounts to 300 PJ and is needed to supply steam and high-temperature heat in ovens (excl. steam cracking). Electricity demand is at 100 PJ and is required for separation processes like electrolysis (e.g. chlorine) and for mechanical energy like compressing.

Today, the petrochemical industry is integrated in many cases in refinery complexes. Exemplary sites in Europe are Rotterdam (Netherlands), Cologne (Germany), Plock (Poland) or Tarragona (Spain).

Existing scenario literature on the future of petrochemical production – if addressing carbon neutrality at all – does not take into account the possible role of existing assets in the vertical integrated clusters and the phase-out of conventional crude oil refinery operations in the transformation of the sector.

With this paper we would like to contribute to a better understanding of the change process on the way to carbon neutrality and the possible role that specific clusters and regions may take. We present an approach to derive scenarios for the transition of the petrochemical industry bottom-up, i.e. considering today's production stock and infrastructures and describing reinvestment in conventional or new technologies. The cost-optimization model used to develop the scenarios describes at which sites investments of industry in the production stock could take place in the future. Around 50 types of products, the related production processes and the respective sites have been collected in a database. The processes included cover the production chain from platform chemicals via intermediates to polymers. Pipelines allowing for efficient exchange of feedstock and platform chemicals between sites are taken into account as well. The model draws on this data to simulate capacity change at individual plants as well as plant utilization. Thus a future European production network for petrochemicals with flows between the different sites and steps of the value chain can be sketched.

In this paper we present and compare results from two scenarios: one "Producer Driven" scenario with unmitigated demand growth for plastics, and one "Circular Economy" scenario with decreasing demand and lower waste generation. The scenarios reveal how, in both cases, an electrification strategy could be implemented by European industry over time with minimized societal costs.

Finally, we discuss possible implications for the chemical industry, the energy system and national or regional governments.

System analysis and modelling framework

STANDARD PRODUCTION ROUTES FOR PLATFORM CHEMICALS

The bulk of today's new polymer production (i.e. not recycled plastics) can be derived from a few so-called platform chemicals. These are olefins (ethylene, propylene and butadiene), aromatics (benzene, toluene and xylene), chlorine, ammonia and methanol. Recyclates from mechanical recycling of plastic waste are an increasing source for polymers used in the plastics converting industries. So-called chemical recycling does not play a significant role yet, but several pilot plants are operated in Europe. Chemical recycling can supply so-called monomers or platform chemicals or a synthesis gas of carbon monoxide and hydrogen. Today's standard routes for the production of platform chemicals are presented in Table 1 with regard to energy and feedstock use as well as emissions and economic parameters like capex and opex. Not shown in the table, another very important source of aromatics today is the catalytic reforming of heavy naphtha in refineries. As aromatics use in gasoline is very restricted by regulation, these aromatics are often used as a chemical feedstock. In the scenarios described in this paper catalytic reforming was not explicitly modelled.

We use a production stock database that was developed during recent years at the Wuppertal Institute. It accounts for existing production stocks for basic materials, intermediate products as well as polymers. For basic materials producing stock (see the processes listed above) individual plant age is accounted. All processes listed in the database are described by their annual production capacity and their specific educt and final energy demands according to literature values. Each of the plants listed is linked to a specific site.

The database contains around 1,000 items of the chemical industry in the EU27+3. For the analysis in the paper at hand we focused on 50 kinds of petrochemical processes and also aggregated some of the sites to "clusters" to reduce the complexity for the solver we used in the optimization procedure. We consider 155 production clusters, hosting 664 production plants in 2020. Sixty of those clusters are located at harbours and as such they also host import terminals for feedstock and HVCs.

Table 1. State-of-the-art production routes for platform chemicals [source: own calculations based on Ren (2009), Bazzanella/Ausfelder (2017), IEA (2009)].

process	educts	products	relevance today *EU production in [Mt/a]*	feedstock *(educt use*) [t/HVC]*	energy use *[GJ/ t HVC]*	CO_2 emissions *[t CO_2/ t HVC], incl. EOL*	capex *[k€/ (t HVC *a)]*
naphtha steam cracking	light naphtha	olefins, aromatics	not reported	1.3	–****)	4.3*****)	0.6
ethane steam cracking	ethane	ethylene, propylene	not reported	1.3	–****)	3.8	1.4
propane dehydrogenation	propane	propylene	0.4	1.3	–****)	3.9	0.7
FCC	heavy gas oil (HGO)	propylene (gasoline, diesel etc.)	7.2***)	5.0	0.5	3.3*****)	*not considered*
chlorine electrolysis	sodium chloride	chlorine (hydrogen)	8.0**)		10-12	–	
ammonia synthesis (+steam reforming of natural gas)	(natural gas →) hydrogen, nitrogen	ammonia	15.2**)		0.1	1.8******)	
methanol synthesis (+steam reforming of natural gas)	(natural gas →) CO, hydrogen	methanol	1.3**)		10	2.0	

*) *"HVC" stands for high-value chemicals and these are defined as the target products (e.g. olefins and aromatics). By-products are indicated in the products column in brackets and are not counted as HVC.*

**) *Only part of the production is used for polymer production.*

***) *Estimation.*

****) *Included in feedstock use.*

*****) *Including emission allocations from oil refining.*

******) *Including process related emissions from hydrogen production via methane steam reforming.*

MODEL DESIGN

The Wuppertal WISEE model framework consists of a database of temporally and geographically detailed process and economic parameters feeding into three main modules (material stock, dispatch, and stock invest modules, respectively) which are in turn linked together to generate temporally and geographically differentiated installed production capacities, energy and feedstock flows, and CO_2 emissions. We use this framework to derive possible pathways on how to achieve carbon looping in the plastics sector. Figure 1 shows the WISEE framework and its use to derive the scenarios described in this paper.

The production of plastics, with the associated demands for feedstock and energy as well as CO_2 emissions, is derived in several steps:

- Plastic demand (by plastic sorts) is derived for a BAU case by extrapolating the trend of plastic use intensity in the so-called "conversion sectors", i.e. the economic sectors taking in plastics and converting them into products like cars or buildings. Other demand pathways can be derived by assumptions built on top of the BAU development (i.e. savings of plastic with x % for a specific product group).
- Plastic waste "supply" is calculated by a plastic stock model (WISEE ms). Annual plastic stock intake (previous step) and assumptions on the lifetime of the several product groups (including a distribution) drive the model.
- Assumptions on the usability of the waste for mechanical recycling as well as possible recyclates intake of the different sectors result in mechanical recycling rates and the amount of new polymers needed by matching supply and demand in each year until the end of the scenario horizon (i.e. the year 2050).
- New polymers can be produced by the production stock available in a specific scenario year. The WISEE edm-I module is a linear optimization model minimizing overall costs. It "decides" if the remaining production stock from earlier periods is sufficient or if new investment is needed to meet demand and also where in Europe such new investment could be integrated in an optimal way into the production networks. The model may also idle existing production stock (before having reached the end of technical lifetime) favouring other technologies that produce more efficiently.
- In the last step WISEE edm-D calculates full energy and CO_2 balances for each site considered in the EU27+3 based on the utilization rates of production stock derived by edm-I. edm-D also accounts for steam and hydrogen integration at sites (i.e. the use of steam or hydrogen by-production in other processes consuming steam or H_2). Energy demand for mechanical recycling is not accounted in the model.

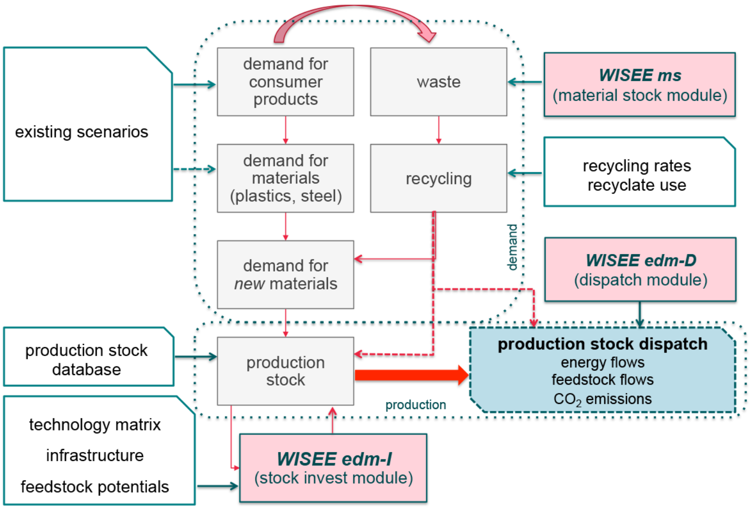

Figure 1. Modelling plastics with the WISEE model framework [source: Wuppertal Institute].

Scenario design: Producer Driven (PD) vs. Circular Economy (CE) scenario

Preceding the quantitative modelling work, qualitative scenarios were co-created with experts and stakeholders during workshops. This input helped shape and plausibility check the calculations for the future of the petrochemical industry.

We developed and modelled two alternative storylines with WISEE. The exogenous parameters, or drivers, to the model differ in distinctive ways between the two scenarios.

EXOGENOUS PARAMETER "DEMAND FOR PLASTICS"

In both scenarios the demand for plastics is driven by the demand of plastic converters in the EU27+3 (EU plus UK, Norway and Switzerland). The sectors that we identify as most relevant are food industry, automotive, construction sector as well as electrical equipment and electronics (see e.g. Plastics Europe 2019). We assume the structure of polymer demand within the sectors to be stable, i.e. the modelling cannot account for possible substitution effects between different polymers in the future. Nevertheless, the projection of demand for the several polymers differs because of differing structure of demand and differing plastic demand developments between the sectors. Another issue changing demand structure for polymers in the future are the different recycling rates and the different potentials of the conversions sectors to use recyclates from mechanical recycling.

In the Producer Driven scenario plastics *demand* follows a business-as-usual pathway. In order to derive a future development, we extrapolate the historical trends of plastic intensity (relationship between plastic demand of this sector in tons and real gross value added of the sector) to the future. We take GVA development from the PRIMES scenarios (Capros et al. 2016). We assume sector GVA change rates for Norway and Switzerland to be the same as for the (former) EU28 (incl. the UK).

The Circular Economy scenario includes assumptions on a considerable reduction of plastic use.

To achieve this potential the ways in which we use plastics, and the products and structures made from it, are expected to change over the coming decades. A wide range of demand-side opportunities are seized so that less material input can yield the same economic benefits. Key strategies identified include material efficiency, sharing business models and increased product lifetimes (e.g. through design for reuse). Regarding packaging, we assume a reduction of 50 % compared to the PD scenario. In such a case 2050's plastics demand for packaging would be at the level of 1997 or 70 % of that in 2017. In the construction sector, lightweight design, improved floor space utilisation, extending building lifetimes and re-using buildings and building components is expected to reduce material demand. For a documentation of assumptions in regard to plastics use please see Schneider et al. (2020). As a result, demand in the Circular Economy scenario is actually *lower* in 2050 than it is today.

EXOGENOUS PARAMETERS "CO_2 PRICE" AND "CO_2 EMISSION FACTORS"

Both scenarios feature a mainly CO_2 price driven development with cross-sectoral cooperation. The projection of the IEA's (2018b) Sustainable Development Scenario in the World Energy Outlook foresees a CO_2 price of $63/t in 2025 and of $140/t in 2040 (equivalent to €128/t). To reach carbon neutrality in the model we assume a carbon price of €200/t in 2040 for both scenarios. For 2050 we use a prohibitively high price of €1,000/t CO_2 as model input. It has to be stressed that such a high price is actually not needed to achieve carbon neutrality but just a technical input for the model, which we could have also achieved with an emission cap of zero for 2050. We did not explicitly regard possible synergies with the fuel sector, which is similar to the approach taken in recent roadmap papers of the chemical industry (VCI 2019) and the study by Dechema (Bazzanella/Ausfelder 2017), although the joint production of naphtha and gasoil in a Fischer-Tropsch process could probably offer such synergies.

CO_2 emission factors in both scenarios include end-of-life (EOL) emissions for the plastics produced from fossil feedstock. Plastics from waste are considered as having no CO_2 burden since the EOL emissions are already allocated to the plastics in the first cycle year when fossil feedstock is extracted and refined. We assume consequently that biomass use as a feedstock does not have negative emissions but is CO_2 neutral.

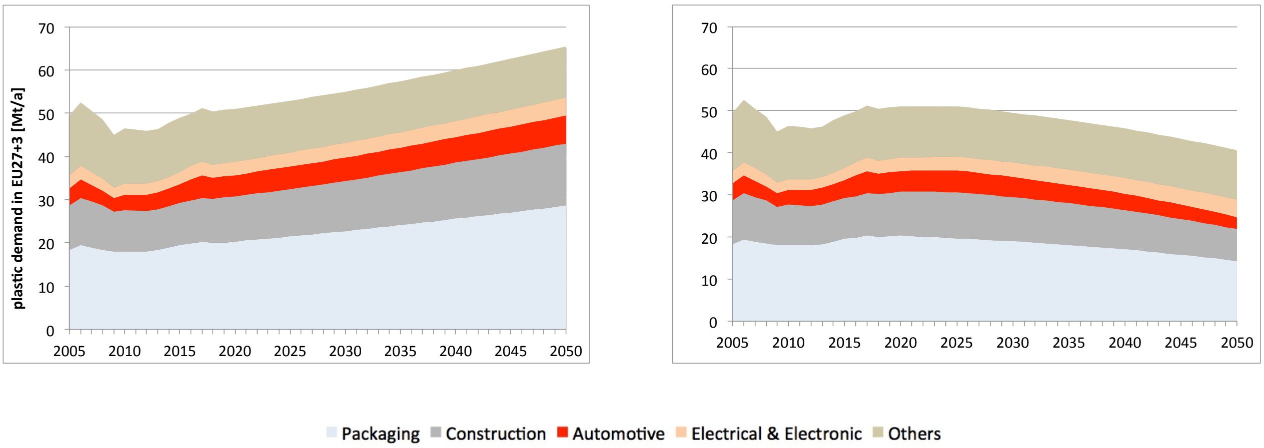

Figure 2. Development of plastics demand in the key plastic converting sectors in the "producer driven" (left) and "circular economy" (right) scenarios [source: own calculation].

Table 2. Emission factors used for the model calculations [source: own assumptions, for EOL based on stoichiometric calculations].

activity	unit	2020	2030	2040	2050
naphtha (EOL)	t/t	3.1	3.1	3.1	0
ethane (EOL)	t/t	2.9	2.9	2.9	–
propane (EOL)	t/t	3.0	3.0	3.0	–
electricity (indirect)	t/GJ	93	75	0	0
steam (indirect)	t/GJ	62	56	19	0
HT heat (direct)	t/GJ	56	56	28	0

Emission factors used to calculate emissions related to energy use in the manufacturing process are documented in the following table.

EXOGENOUS PARAMETER "WASTE STREAMS"

The WISEE Plastic Stock model (WISEE ms) derives available polymer waste flows in Europe over time, fed in turn as exogenous parameters into the EDM-I model. After accounting for losses, low qualities and exports remaining polymer waste streams are available for mechanical or chemical recycling.

Mechanical recycling is prioritized over chemical recycling for energy efficiency reasons. Therefore we used the techno-economic potentials for mechanical recycling assessed in other studies (Material Economics 2018, Material Economics 2019). Challenges in mechanical recycling limiting its potentials are mainly fibre degradation and compounds or mixed plastics streams (Ragaert et al. 2017). The difference between total recyclable plastic waste flow and input in mechanical recycling is in principle available for chemical recycling. Actual availability is further reduced by the fact that some waste streams must be deposited as a legal requirement.

For the PD scenario we calculated a potential waste feedstock for chemical recycling of about 24 million tons in 2050 and of 18 Mt in the CE scenario. How much of that potential is then actually used as feedstock in chemical recycling is decided in the *WISEE edm-I* invest model where two chemical recycling routes compete with conventional fossil-based routes, based on cost efficiency.

Growing demand for plastics in the PD scenario cannot be covered by waste, be it by mechanical recycling or chemical recycling – not even in the (theoretical) case where all waste could be recycled. The growing plastics stock requires a permanent inflow of additional hydrocarbon feedstock, losses in the system (exports of waste, thermal treatment) add up additional demand for new feedstock.

The CE case shows a completely different development of plastics demand. With the rapid decrease in demand after 2020 (theoretically) available waste amounts even exceed demand after 2035. Due to losses, low qualities and exports there is however still a need for primary production in this scenario.

EXOGENOUS PARAMETERS "FEEDSTOCK PRICES"

In both scenarios we assume optimistically low hydrogen price for the late 2030s (€1.44/kg in 2040) and the 2040s (€1.23/kg in 2050). This represents the lower end of a plausible range from €1.65 to €1.80/kg in 2030 and €1.23 to €1.34/kg in the 2040s and 2050s. In this scenario methanol could be available at ARA[1] or Mediterranean ports at €489/t (2040) and €457 in 2050 (includ-

1. ARA stands for the three North Sea ports of Amsterdam, Rotterdam and Antwerp.

Table 3. New production routes for platform chemicals [source: own compilation based on Schneider et al. (2019), Zhang/El-Halwagi (2017), Bazzanella/Ausfelder (2017), Fivga/Dimitriou (2018), Pérez-Fortes et al. (2016), Collodi (2017), dena (2017), Amirkhas (2006), Thunman et al. (2018), Thunman et al. (2019)]

process	educts	products	feedstock (educt) use [t/HVC*)]	energy use [GJ/ t HVC]	capex [k€/ (t HVC *a)]
plastic waste pyrolysis	sorted plastic waste	pyrolysis oil	1.6	3.5	0.5
plastic waste gasification (+MeOH synthesis)	unsorted plastic waste	(syngas →) methanol	0.4	10	0.9**)
electric steam cracking	naphtha (ethane)	olefins, aromatics	1.3 (ethane: 1.2)	9	0.6 (ethane: 1.4)
biogenic carbon processing to methanol	black liquor	methanol	3.3	19	1.1***)
DAC based methanol	CO_2, hydrogen	methanol	1.4 (CO_2) + 0.2 (H_2)	33	1.3
MtO	methanol	ethylene, propylene	2.7	0.1	0.9
MtA	methanol	para-xylene, toluene, benzene	4.3	0.1	1.1

*) *"HVC" stands for high-value chemicals and these are defined as the target products (e.g. olefins and aromatics).*

**) *Excluding capex for H_2O electrolysis.*

***) *Including capex for H_2O electrolysis.*

ing shipping costs of €12/t). However, under worse conditions hydrogen supply costs could be at the higher end of the range. Higher hydrogen costs would however not change Producer Driven modelling results much. Technologies with rather high operational costs are needed in this high plastics demand scenario and they all have similar specific hydrogen requirements.[2] The CE scenario may be more sensitive to higher hydrogen prices.

An additional important assumption for both scenarios is that fossil feedstock will be available at prices comparable to today in the future. Although the deep decarbonisation scenarios of the IEA (2018b) show a drop in crude oil prices compared to today due to rather stable global transport fuel demand, the supply costs for shale gas-based ethane and propane could be higher in the future than today. These are today's fossil benchmark feedstock for olefin investments (ethane crackers and propane dehydrogenation) and the demand for it could grow considerably mainly due to growing global demand for plastics (especially in Asia and Africa). If ethane and propane prices do increase considerably this could (together with lower hydrogen supply cost) result in higher and earlier investments in waste based and DAC based production routes in Europe.

LOW CARBON TECHNOLOGY OPTIONS

The same technology options are available in both scenarios to meet the future demand for monomers, whose dynamics and absolute level greatly varies by design between the Producer Driven and Circular Economy scenarios. These novel technology routes rely on waste or biogenic feedstock – in the long run even on CO_2 from the atmosphere. These technologies all have the potential of being operated carbon neutral and are presented in Table 3 with their respective feedstock and energy demands as well as specific investment requirements.

The two chemical recycling routes are, on the one hand, the pyrolysis of plastic waste with pyrolysis oil as a feedstock than can be converted in steam crackers to platform chemicals and, on the other hand, gasification of plastic waste to produce a syngas than can be converted to methanol. Methanol can be further processed via the MTO process to olefins and via MTA process to aromatics (see above). The first route requires cleaner waste whereas the latter one may also cope with contaminated waste (Ragaert et al. 2017). Following Material Economics (2019) it was assumed that 50 % of future plastic waste is available for the first route, which is cheaper and can easier be phased in into existing production systems, with steam crackers being already available.

Modelling results

TECHNOLOGY MIX

The Producer Driven scenario foresees no plastic demand reduction measures. Plastic demand develops "business-as-usual". Mechanical recycling rates and recyclates input in plastics conversion increase but demand for new plastics produced from monomers still increases as well. This coupled with the assumption of high CO_2 prices result in high exploitation rates for waste as a plastic feedstock over time. In contrast, the supply of platform chemicals in the Circular Economy scenario is marked by a decrease in capacity and production due to lower demand and also to higher recyclate use. Figure 3 shows the different dynamics in terms of installed production capacity and utilization in both scenarios.

2. Very high hydrogen import prices and relative low EU electricity and hydrogen prices could increase the share of electric cracking with a carbon recycling of the by-products resulting in lower methanol or green naphtha imports.

In the PD scenario, especially inland sites require new feedstock. As the refineries phase out (in the model according to age and technical lifetime of the atmospheric distillation units), these sites lose their naphtha supply and need a new feedstock. Ethane or propane is only available to low cost at coastal sites, so inland sites start to import olefins (especially ethylene via pipeline) or build up chemical recycling plants as soon as the CO_2 price burden on fossil feedstock (incl. end-of-life emissions) is high enough to meet the threshold.

The plastic waste pyrolysis route is already economically viable in 2030. At this date, already 10 million tons of plastic waste are treated via this route, which represents 100 % of the assumed potential. The very early adopters are the sites with existing flexible steam crackers like Grangemouth (UK), Gonfreville (France) or Terneuzen (Netherlands). In 2030 the big inland chemical parks in Geleen (Netherlands) and North Cologne (Cologne/Dormagen, Germany) as well as Brindisi (Italy) adapt their steam cracker capacities to flexible feedstock supply and build up pyrolysis plants. Figure 3 shows that naphtha steam crackers are being idled to a great extent already in 2030. Only half of the capacity is utilized due to relatively high feedstock costs. In the CE scenario as well, many crackers are rebuilt in the 2020s and 2030s as flexible crackers. Thus, they can take up ethane in the mid-term but also run on pyrolysis oil from plastic waste in the long-run.

The phasing out of refinery propylene production from FCC results in a shortage of this olefin. Today, one propane dehydrogenation plant is running at Tarragona (Spain) and three other ones are under construction. Around 2030 other projects follow and fill the propylene gap until 2040. But due to being captive to a fossil feedstock these plants are not operated any more after 2040.

Waste not applicable in pyrolysis plants due to contaminations or very mixed fractions is treated in gasification plants to produce methanol. Such complex production requires several additional process steps including the subsequent processing of methanol-to-olefins or methanol-to-aromatics step. Investments in MTO and MTA start around 2040 with a higher CO_2 price. By that time methanol as by-product from the pulp and paper industry as well as from sweet renewable electricity spots (DAC based) is available in our scenario.

FEEDSTOCK AND ENERGY ACCOUNTING

Figure 4 shows the full energy balance for the plastics sector in the EU27+3 in both scenarios. It comprises nearly all primary energy use including the feedstock. Delta between energy use and the energy content of the products is the conversion loss. Today, this loss accounts to around 40 %. In the future, with more sophisticated procedures it could easily reach 50 %. It has to be stressed that the system boundary here does neither include today's losses in refineries when supplying naphtha nor methanol production in the future. If they are taken into account as well losses are even higher.

Methanol from pulping enters the market in 2040. At that time plastic waste gasification also becomes a source used to produce methanol. Respective methanol processing capacities are built-up as well as shown in the previous section. The CE case does without the two most expensive options to supply feedstock, which are DAC-based methanol import and methanol-based on by-products from electrified steam crackers. However, naphtha imports are still necessary in 2050 especially for butadiene supply by naphtha-based steam cracking.

The more complex (and thus more lossy) feedstock and process routes needed in the latter years (with very high CO_2 prices) in the PD scenario explain why the energy use increases much faster than polymer production. In the CE scenario this aspect is much less relevant although energy use slightly increases while polymer production decreases.

EMISSION ACCOUNTING

Figure 5 displays the CO_2 balance for the whole plastic sector in both scenarios. CO_2 emission reduction in 2030 reaches around 26 % and 32 % compared to 2015 in the PD and CE scenarios, respectively. In both cases emissions decrease much faster afterwards. The decline is steeper in the CE case, however. 57 % and almost 70 % reductions are achieved in 2040 in the PD and CE scenarios, respectively. Higher cuts would be possible if green naphtha would be imported instead of fossil feedstock. In 2040, with a CO_2 price of €200/t, it is available at a price of €1,900/t, which is not competitive yet compared to the import of fossil naphtha. In 2050 renewable naphtha is available at a price of €1,400/t and all remaining naphtha import is then from renewable sources. As all other feedstock comes

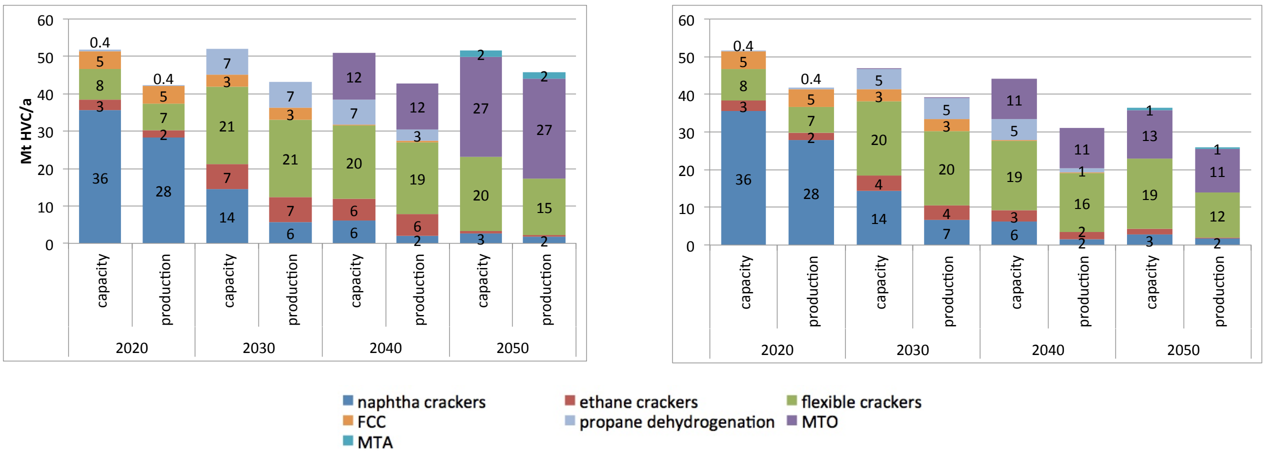

Figure 3. HVC capacities and production in the PD (left) and CE (right) scenarios [source: own calculations].

either from waste or from renewable sources as well the system is then CO_2 neutral.

GEOGRAPHICAL CHARACTERISTICS OF THE RESULTS

The invest model optimizes investment in new technologies and stock and the use of individual production stock on a site-level ("dispatch"). In our model transport costs to and from specific sites, existing production stock and its individual phase-out due to plant age drive the change in spatial patterns. A change in plastic demand (e.g. due to reduction of packaging in the CE scenario) might also have spatial impacts. So a reduction in PE-LD use will particularly hit sites with olefin production stock that is vertically integrated onsite with PE-LD production.

Figure 6 shows where the production of HVC occurs in both scenarios in 2050. In the Producer Driven scenario (i.e. high-production level) today's chemical clusters are still there. The concentration of cracking facilities in Western Europe around the ARA ports is striking. This is mainly due to the complex value chains there that depend on various platform products (including aromatics). Cracking offers synergistic production in this case. Other sites depending on ethylene and propylene only make use of the emerging availability of methanol as renewable feedstock and rely on MTO plants.

In the Circular Economy scenario (i.e. with shrinking demand for plastics) only the most efficient clusters survive. The so-called "petrochemical triangle" of Flanders, South Holland and Rhine-Ruhr with the three vertices being Antwerp, Rotterdam and Rhine/Ruhr has a 50 % share in production capacities today and even increases its share. Many other production sites are mothballed or scaled down.

Other heavy industry sites are rather single sites and not clusters. Most often they have a clear focus on one or two production routes. Locations at the coast will not lose their competitive advantage over inland sites. They are in general much more flexible in their access to new energy carriers or feedstock, which could be observed in recent years for steam cracking sites at the coast which were able to react to very low prices for ethane from the U.S. and converted their plants to flexible crackers.

Electricity and hydrogen use in 2050 also unmistakably show some clusters. The most prominent one consists of the Flanders region, South Holland and Western Germany ("petrochemical triangle"). Another important cluster is the Rhône delta around Marseille. Both regions have a strong diversity in heavy industries and differentiated value chains, especially in the plastics sector. If the structure in plastics demand (namely the portfolio of plastics sorts) does not change too much in favour of new plastic sorts, these clusters will remain robust because of the high synergies they provide.

COSTS

We calculated one reference case for the PD and one for the CE scenario, respectively, to derive conclusions on costs. In each reference case polymer production is as high as in the cor-

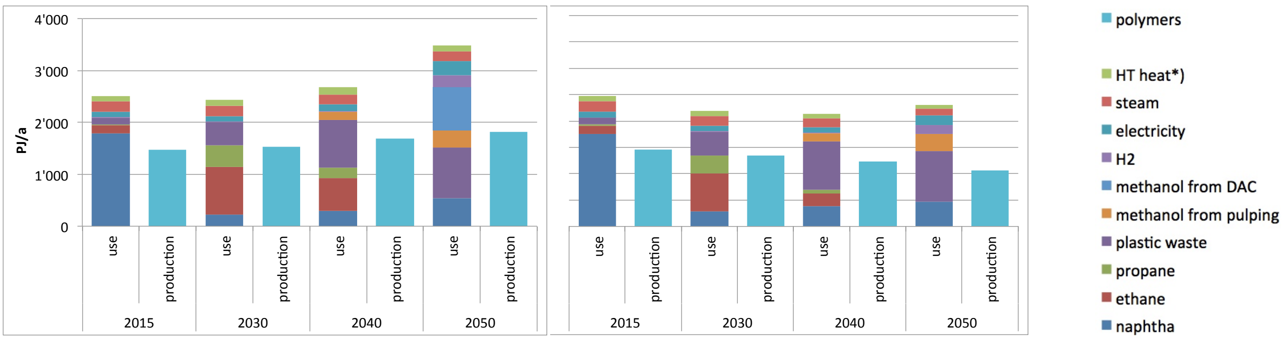

Figure 4. Energy balance for plastics production in the EU27+3 (including feedstock use) in the PD (left) and CE (right) scenarios [source: own calculation].
**) HT heat stands for "high-temperature heat" supplied by industrial ovens.*

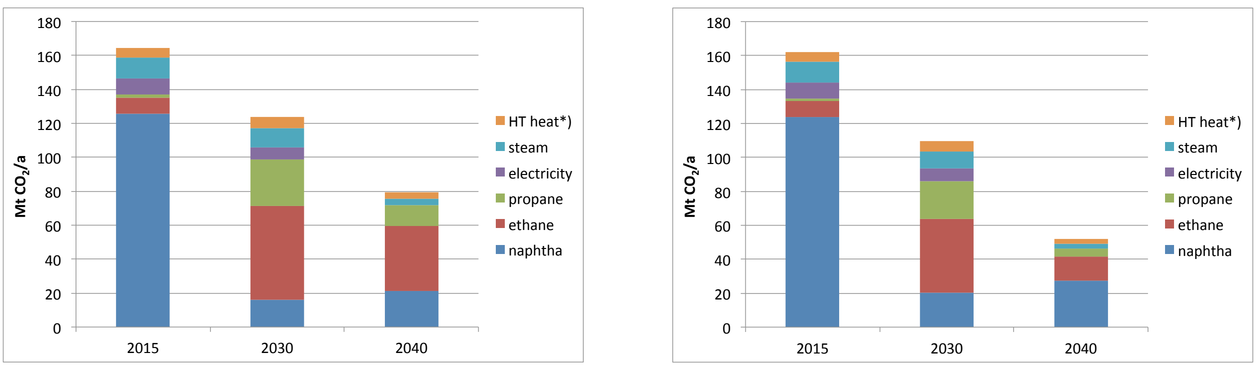

Figure 5. CO_2 emissions related to plastics production in the EU27+3 in the PD (left) and CE (right) scenarios [source: own calculations].
**) HT heat stands for "high-temperature heat" supplied by industrial ovens.*

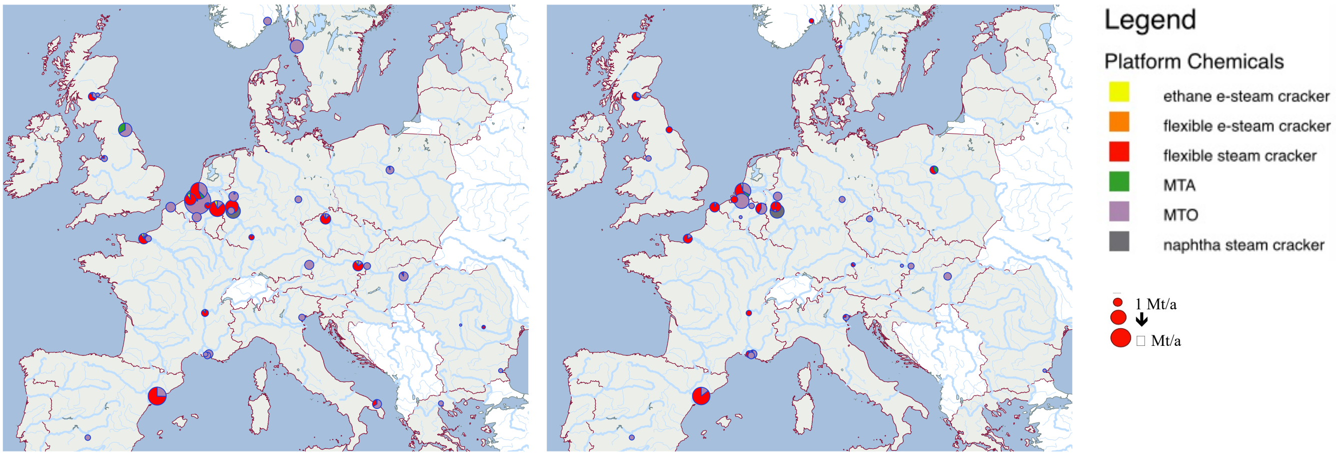

Figure 6. Map on HVC production in 2050 in the PD (left) and CE (right) scenarios [source: own calculation].

responding PD or CE scenario. Capital cost (capex) and operational cost (opex) amounts for downstream operations (to produce intermediates and polymers) are equal between the main scenarios and the corresponding references. According to Material Economics (2019) these amounts are at a level of €400 per ton of plastic compared to €800 or more for the production of the basic materials.

The main difference between the PD and CE scenarios and their respective references is the level of the CO_2 price: in the reference case the price is considerably lower. We refer here to the World Energy Outlook (IEA 2018b) again, but use the values for the "current policies" scenario. Converted to Euros, the CO_2 price pathway until 2040 reaches €20/t in 2020, €27/t in 2030 and €35/t in 2040. With an extrapolation to 2050 we end up at €42/t. Another difference is that methanol from European biomass (i.e. black liquor from chemical pulping) is not available in the reference case. Plastic waste for chemical recycling on the other hand is available in the reference as well and can thus be used. As the diffusion of new technologies is mainly cost driven in the scenarios it differs between the two scenarios and their respective reference cases. Diffusion of new technologies is not prohibited in the reference case, but is actually at much lower pace. Many of the costly technologies (like gasification of plastic waste) are not used at all in the reference case and the potential for chemical recycling is thus only partly used resulting in more primary production from fossil resources.

These differences account for the cost differentials shown below.[3] Table 4 and Table 5 show a cost comparison between our two scenarios and the respective references. To ensure comparability we did not include costs related to CO_2 emissions into the comparison, as they are no real societal costs.

Table 4 indicates that the total discounted cost differential between the PD scenario and its reference is only €102 billion for the whole modelling period (i.e. from 2015 until 2055). This rather low amount is due to the fact that most of the extra costs occur at later points in time, where the discount rate of 5 % has a great impact. So in the latest modelling decade (2045–2055) actual (non discounted) extra cost flows are much higher with more than €300 billion. During this decade society has to pay €638 more for one ton of polymer than in the reference case (see last column in Table 4). Compared to the CO_2 emission reduction achieved in this decade we end up with mean mitigation costs of €150/t CO_2 in 2040 and €253/t CO_2 in 2050 – which is considerably lower than the respective CO_2 price of €200 in 2040 and the technical assumption of €1,000/t in 2050 in the PD scenario (the comparison still holds when looking at the slightly lower CO_2 price differential between PD scenario and its reference, that is €165 in 2040 and €958 in 2050). It can thus be seen that mean societal costs per ton of CO_2 are much lower than the CO_2 price, which is logical as the CO_2 price represents a marginal cost price.

In Table 5 differential costs compared to the reference are in the period 2035–2045 even higher than in the PD scenario. This does not necessarily mean that the total costs per ton of polymer are higher than in the PD scenario, despite €211/t polymer being higher than €148/t in the CE and PD scenarios, respectively (last column of Table 5). Indeed, in the PD case chemical industry "profits" from a higher availability of plastic waste, which can be seen as an investment of prior time periods. The total discounted differential costs are however much lower in the CE scenario. The most important reason is that chemical industry can do without the most expensive technical option to use imported methanol derived from direct air capture and water electrolysis in the latest decade.

Discussion

One should keep in mind that the novel production pathways that we included in the technology matrix of the model represent only a fraction of possible technologies. Other future technologies might offer better economic suitably to the demand structure showed in our scenarios or perform better with regard to energy efficiency. Therefore, the mix of technology pathways regarding general technology classes (e.g. steam cracking vs. MTO) might have been different had other technology types been considered. The technology pathways delineated by the model can however be understood as prototypical for technology groups and the mix derived by the model is not only consistent with respect to the assumptions taken but also realistic at least in qualitative terms.

3. We cannot analyse the reference cases in depth here, but may add that plastic waste pyrolysis is one "low carbon" technology that is also used in the reference cases, albeit to a lower extent than in the scenarios aiming at carbon neutrality.

Table 4. Differential costs and CO_2 mitigation costs in the PD scenario vs. reference [source: own calculations].

	total cost deviation vs. reference		polymer production	delta CO_2 vs. reference	CO_2 mitigation costs vs. reference	specific extra production costs vs. reference
	bill. $€_{2015}$; *discounted*	bill. $€_{2015}$; *not discounted*	bill. tons of polymer	bill. tons of CO_2	$€_{2015}$/t of CO_2; *not discounted*	$€_{2015}$/t of polymer; *not discounted*
period 2015–2025	0.0	0.0	0.41	0.0	–	0
period 2025–2035	0.1	0.2	0.43	0.0	–	1
period 2035–2045	27	70	0.48	-0.5	150	148
period 2045–2055	75	326	0.51	-1.3	253	638
total period 2015–2055	102		1.84	-1.8		

Table 5. Differential costs and CO_2 mitigation costs in the CE scenario vs. reference [source: own calculations].

	total cost deviation vs. reference		polymer production	delta CO_2 vs. reference	CO_2 mitigation costs vs. reference	specific extra production costs vs. reference
	bill. $€_{2015}$; *discounted*	bill. $€_{2015}$; *not discounted*	bill. tons of polymer	bill. tons of CO_2	$€_{2015}$/t of CO_2; *not discounted*	$€_{2015}$/t of polymer; *not discounted*
period 2015–2025	0	0.0	0.41	0.0	–	–
period 2025–2035	0	0.2	0.38	0.0	–	0.4
period 2035–2045	28	74	0.35	-0.4	178	211
period 2045–2055	43	187	0.30	-0.8	237	630
total period 2015–2055	71		1.4	-1.2		

We want to stress that the development described in the scenarios requires a lot of renewable energy supply, notably electricity and electricity-derived hydrogen. The energy supply system could not be modelled alongside the industrial system for this paper. However, we considered availability implicitly when making assumptions about the phase-in of technologies and about supply costs of renewable feedstock for the plastics industry.

Other scenario studies for the petrochemical industry with high technology resolution like Bazzanella and Ausfelder (2017) or the recent roadmap study by the German Association of the Chemical Industry (VCI 2019) have not included the energy system either, but show even higher energy demands.

These higher demands can be attributed to several reasons:

- The plastics demand pathway is higher (Bazzanella and Ausfelder 2017).
- The potential of chemical recycling of plastic waste is neglected (Bazzanella and Ausfelder 2017) or rated very low (VCI 2019).
- Potential energy efficiency improvements are rated very conservatively by assuming lifetime extension of existing production stock without major reinvestments (both studies).

Besides the traditional energy supply system, developments in other sectors not explicitly modelled here are expected to affect renewable energy and feedstock availability. An example of a possible synergy is the use of by-products from the pulp and paper industry as assumed in our scenario. The fuel sector on the other hand could be a partner for the chemical industry (like today) but could also turn out as a competitor in the future for the petrochemical industry, both searching for scarce hydrocarbon sources in Europe. Such developments will have an impact on how much European chemical industry will depend on a "backstop technology" pathway like Direct Air Capture (DAC), which is today not a mature technology and which (if achieving maturity) will most probably not be applied in Europe, but in regions with abundant surplus renewable electricity.

Sectoral insights such as that on plastics presented in this paper would greatly benefit from integrated energy and emission scenarios for the whole system (and the whole world). There have been various potential and scenario studies showing that electricity demand at levels shown in our scenarios can be met by techno-economical potentials, but our analysis cannot yet provide insights of the impacts of such scenarios on the electricity system or vice versa.

The actual implementation of a deep decarbonisation requires various new infrastructures and infrastructure adaptation or amendment. Geographical issues around the production system for plastics have been discussed in this paper to some extent and some core infrastructures like the pipelines for chemicals have been explicitly modelled. A thorough infrastructure analysis that takes de-fossilization of heavy industry (including but not limited to the petrochemical sector) into account is necessary. Some first insights for several European heavy industry clusters have been derived in the Climate-KIC funded project "INFRAneeds"[4], which has been conducted during 2019 by Wuppertal Institute and European Climate Foundation.

Quantitative scenario making needs to be better informed about the uptake of innovations and their diffusion. In building our model we could reach a deeper understanding regarding the implementation speed of concrete technology types based on intensive stakeholder and expert discussions. However, this knowledge did not translate yet into actual quantitative improvements of the model itself. An explicit modelling of innovation systems, which could be addressed e.g. by agent-based modelling (ABM), could improve the model. In the present case the actual uptake of innovations can thus not be directly modelled. Instead, the phase-in of new technologies is derived qua assumption (object of discussions in expert workshops) translated as constraints in the model or through simplified economic considerations entered as exogenous parameters in the model. This shortcoming is less relevant when studying, like here, the plastics industry with rather simple systems of only a few agents who typically behave in a very strategic way (even more so for the steel and paper production systems). However, regarding innovations along the value chain including recycling systems and product design (or also the finance sector) agent-based modelling (ABM) could yet offer additional insights.

Conclusions

Circular economy will help to lower electricity demand in almost every country in the EU. A detailed analysis of future energy demands on the EU member state level covering in addition possible future energy demands of the steel and pulp and paper industry can be found in Schneider et al. (2020).

Considering available potentials for inland renewable electricity production in Germany, Austria and Poland, together with the existence in those countries of petrochemical industries (as well as primary steel production) that may require large amounts of green hydrogen in the future, it appears that these three countries in particular need an import strategy for hydrogen to keep their heavy industry alive. The German government has acknowledged the future crucial role for hydrogen in its "industrial strategy" (BMWI 2019) and currently develops a hydrogen strategy for the country and its industry in order to ensure future availability.

Belgium and the Netherlands are countries with relatively low renewable electricity potentials but very strong chemical clusters around the two ports of Antwerp and Rotterdam. Import will be an issue here as well but can be more easily implemented at the ports.

Petrochemical sites in the inland are today under strong economic pressure compared to coastal sites. The major reason for this is cheap ethane from the U.S. flooding the global petrochemical feedstock markets. Coastal sites are able to import ethane directly by ship, whereas inland sites have yet no cheap access to it. Future possible non-fossil alternatives like green naphtha or methanol may be transported via the seaports through existing pipelines into the hinterland in the future. So as soon as the existing infrastructure are adapted to the new feedstocks, inland sites may also have good access. However, inland sites will be always less flexible to react on changing markets than the coastal sites, which will probably be the forerunners in the adoption of new feedstocks at a large scale. Therefore sourcing waste in their local "plastic waste markets" to use in chemical recycling plants seems to be a robust strategy for inland sites to be less dependent on imported feedstock.

4. See the project website at https://wupperinst.org/en/p/wi/p/s/pd/818/.

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